

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 194 °C

Global applicability domain: Inside

Local applicability domain index: 7.69e-01

Confidence level: 5.90e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Sulfameter</div> <div>Measured: 215</div> <div>Predicted: 194</div>	<div>Image not found</div> <div>Sulfamethoxypyridazine</div> <div>Measured: 183</div> <div>Predicted: 189</div>	<div>Image not found</div> <div>Sulfaethoxypyridazine</div> <div>Measured: 183</div> <div>Predicted: 186</div>
<div>Image not found</div> <div>Sulfamethomidine</div> <div>Measured: 146</div> <div>Predicted: 174</div>	<div>Image not found</div> <div>Sulfadimethoxine</div> <div>Measured: 204</div> <div>Predicted: 196</div>	